

**Microbial dechlorination of polychlorinated biphenyls, dibenzo-p-dioxins, and -furans in groundwater
at the Portland Harbor superfund site, Oregon, USA**

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Supporting information

Five figures

One table



Figure S-1. Map of Portland Harbor superfund site showing major known contaminated sites.

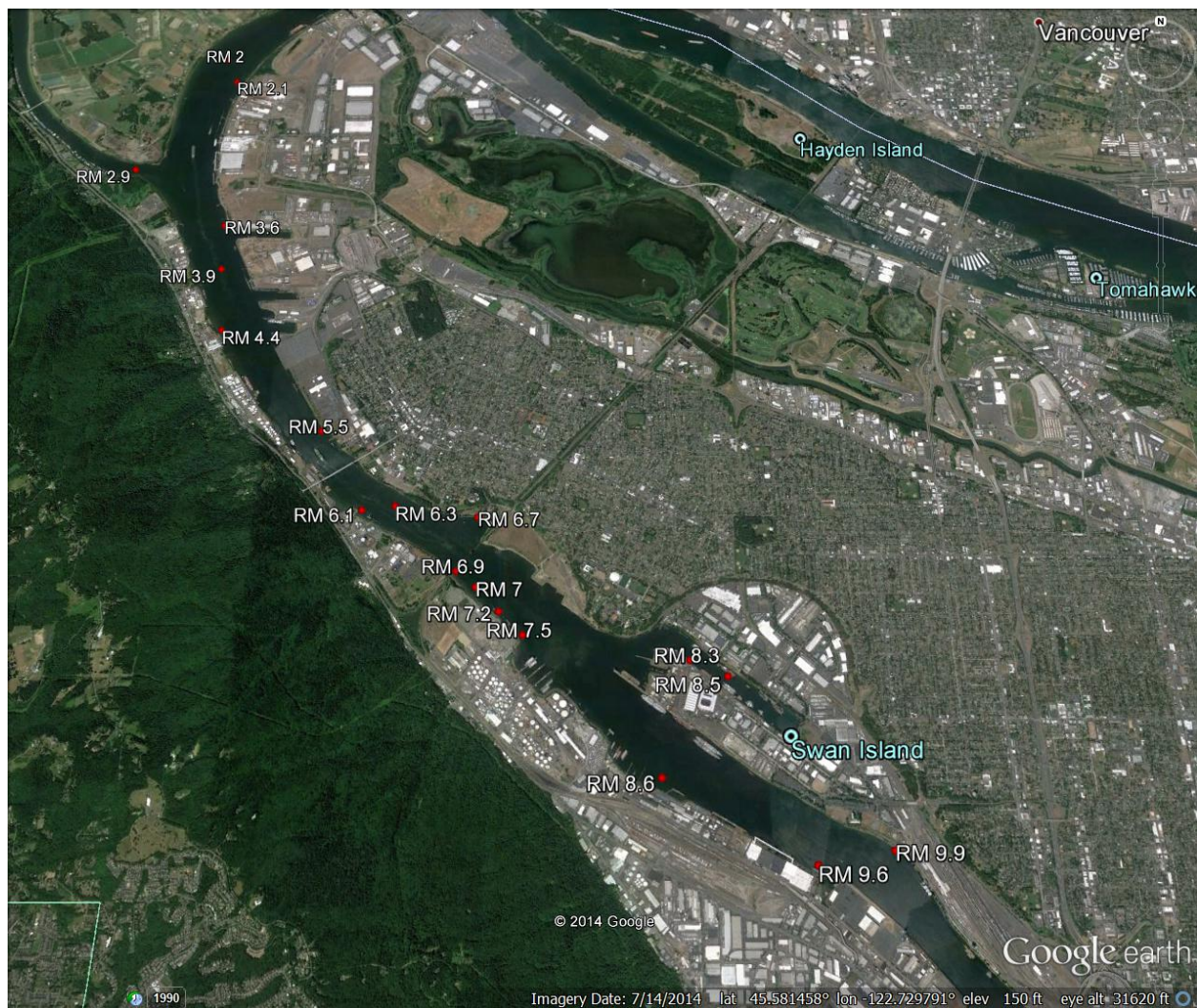


Figure S-2. Map of Portland Harbor showing water sampling sites labeled by river mile (RM). Upstream sites at RM 11 and 15.9 are not shown for clarity. Map drawn with Google earth.

Table S-1. List of congeners used in PMF modeling and coelution patterns.

Sediment (DB-5 column)		Water column (SPB-octyl column)		
PCB004 & 010	PCB129	PCB 4	PCB 88	PCB 197+200
PCB011	PCB130	PCB 6	PCB 90+101+113	PCB 198+199
PCB016 & 032	PCB132 & 161	PCB 8	PCB 92	PCB 202
			PCB	
PCB017	PCB133 & 142	PCB 10	95+100+93+102+98	PCB 203
PCB018	PCB134 & 143	PCB 11	PCB 94	PCB 206
PCB019	PCB135	PCB 15	PCB 103	PCB 209
PCB020 & 021 & 033	PCB136	PCB 16	PCB 105	
PCB022	PCB137	PCB 17	PCB 110+115	
PCB026	PCB138 & 163 & 164	PCB 18+30	PCB 114	
PCB028	PCB139 & 149	PCB 19	PCB 123	
PCB031	PCB141	PCB 20+28	PCB 128+166	
			PCB	
PCB037	PCB144	PCB 21+33	138+163+129+160	
PCB041 & 064 & 071 & 072	PCB146 & 165	PCB 22	PCB 130	
PCB042 & 059	PCB151	PCB 25	PCB 132	
PCB043 & 049	PCB153	PCB 26+29	PCB 134+143	
PCB044	PCB156	PCB 27	PCB 151+135+154	
PCB047	PCB157	PCB 31	PCB 136	
PCB048 & 075	PCB158 & 160	PCB 32	PCB 141	
PCB052 & 069	PCB167	PCB 37	PCB 144	
PCB053	PCB170	PCB 40+41+71	PCB 146	
PCB056 & 060	PCB171	PCB 42	PCB 147+149	
PCB061 & 070	PCB172	PCB 44+65+47	PCB 153+168	
PCB066 & 076	PCB174	PCB 45+51	PCB 156+157	
PCB074	PCB176	PCB 46	PCB 158	
PCB077	PCB177	PCB 48	PCB 164	
PCB082	PCB178	PCB 49+69	PCB 169	
PCB084 & 092	PCB179	PCB 50+53	PCB 170	
PCB085 & 116	PCB180	PCB 52	PCB 171+173	
PCB087 & 117 & 125	PCB182 & 187	PCB 54	PCB 172	
PCB088 & 091	PCB183	PCB 56	PCB 174	
PCB090 & 101	PCB185	PCB 59+62+75	PCB 176	
PCB095 & 098 & 102	PCB189	PCB 60	PCB 177	
PCB097	PCB190	PCB 61+70+76+74	PCB 178	
PCB099	PCB193	PCB 64	PCB 179	
PCB105	PCB194	PCB 66	PCB 180+193	
PCB106 & 118	PCB195	PCB 77	PCB 183+185	
PCB107 & 109	PCB196 & 203	PCB 81	PCB 187	
PCB108 & 112	PCB199	PCB 82	PCB 189	
PCB110	PCB202	PCB 83+99	PCB 190	
PCB114	PCB206	PCB 84	PCB 194	
PCB128 & 162	PCB208	PCB 117+116+85	PCB 195	
		PCB		
	PCB209	108+119+86+97+125+87	PCB 196	

Data matrix details

LODs ranged from 0.1 to 358 pg/g for PCBs in sediment, from 0.00020 to 1.4 pg/L for PCBs in the water column, and from 0.00064 to 3.5 pg/L for PCDD/Fs in water.

Justification for selection of the number of factors

PCBs in sediment

Three, four, five, and six factor solutions were generated. The four factor model was selected. For the four-factor model, all nine seed runs were similar with an RSD of the G matrix of 1.8%. All four of these factors had positive and significant coefficients when the G matrix was regressed against the measured sum of PCBs. In contrast, this regression for the five-factor model revealed one factor with a coefficient that was not significant. Also, for the five factor model, two of the nine seed runs were very different from the other seven. The G-space plots indicated that all factors of the four-factor solution were independent of each other. The agreement (R^2) between measured and modeled concentrations was greater than 0.77 for 80 of 83 peaks. The three peaks/congeners with low R^2 were PCB 206 (0.38), PCB (0.34) and PCB 209 (0.53).

PCBs in water column

Four, five, six, and seven factor solutions were generated. The five factor model was selected. The five factor solution had low RSD of the G matrix (0.43%). The six factor model had two outliers among the nine seed runs. Although both the five and six factor models gave positive and significant coefficients for all factors when the G matrixes were regressed against the measured sum of PCBs, two of the factors in the six-factor model were similar in fingerprint (both resembled Aroclor 1260). Therefore the five factor model was selected. The agreement (R^2) between measured and modeled concentrations was greater than 0.7 for 85 of 90 peaks. The peaks/congeners that were not well modeled were PCB 11 (R^2 = 0.51), PCB 81 (0.24), PCB 123 (0.18), PCB 169 (0.027), and PCB 209 (0.40). Note that PCBs 81, 123, and 169 were included in the data matrix despite low concentrations because they are dioxin-like congeners. The G space plots for the five factor model showed strong correlation between factors W2 and W5, but this was because the regression was dominated by the seven samples with the highest PCB concentrations, all of which were collected at Willamette Cove. When the nine samples collected at Willamette Cove were removed, all of the factors were independent of each other.

PCBs and PCDD/Fs in the water column

Four, five, six, seven, and eight factor solutions were generated. The seven factor model was selected. The six and eight factor models did not converge on a robust solution, with the nine seed runs generating at least three distinct solutions. In contrast, for the seven factor solution, eight of the nine seed runs were in good agreement with each other (RSD of the G matrix = 1.4%). All seven factors yielded positive and significant coefficients in the regression of the G matrix versus the sum of analytes, and all seven were independent of each other. The agreement between measured and modeled

concentrations was greater than 0.7 for 73 of 77 analytes. Analytes with low R^2 values were 1,2,3,7,8,9-HxCDD, 1,2,3,7,8-PCDD, and 2,3,4,6,7,8-HxCDF, all of which had R^2 values greater than 0.65, and PCB 126, a dioxin-like congener. As with the solution for PCBs in the water column, the seven factors were independent of each other when the nine samples from Willamette Cove were excluded.

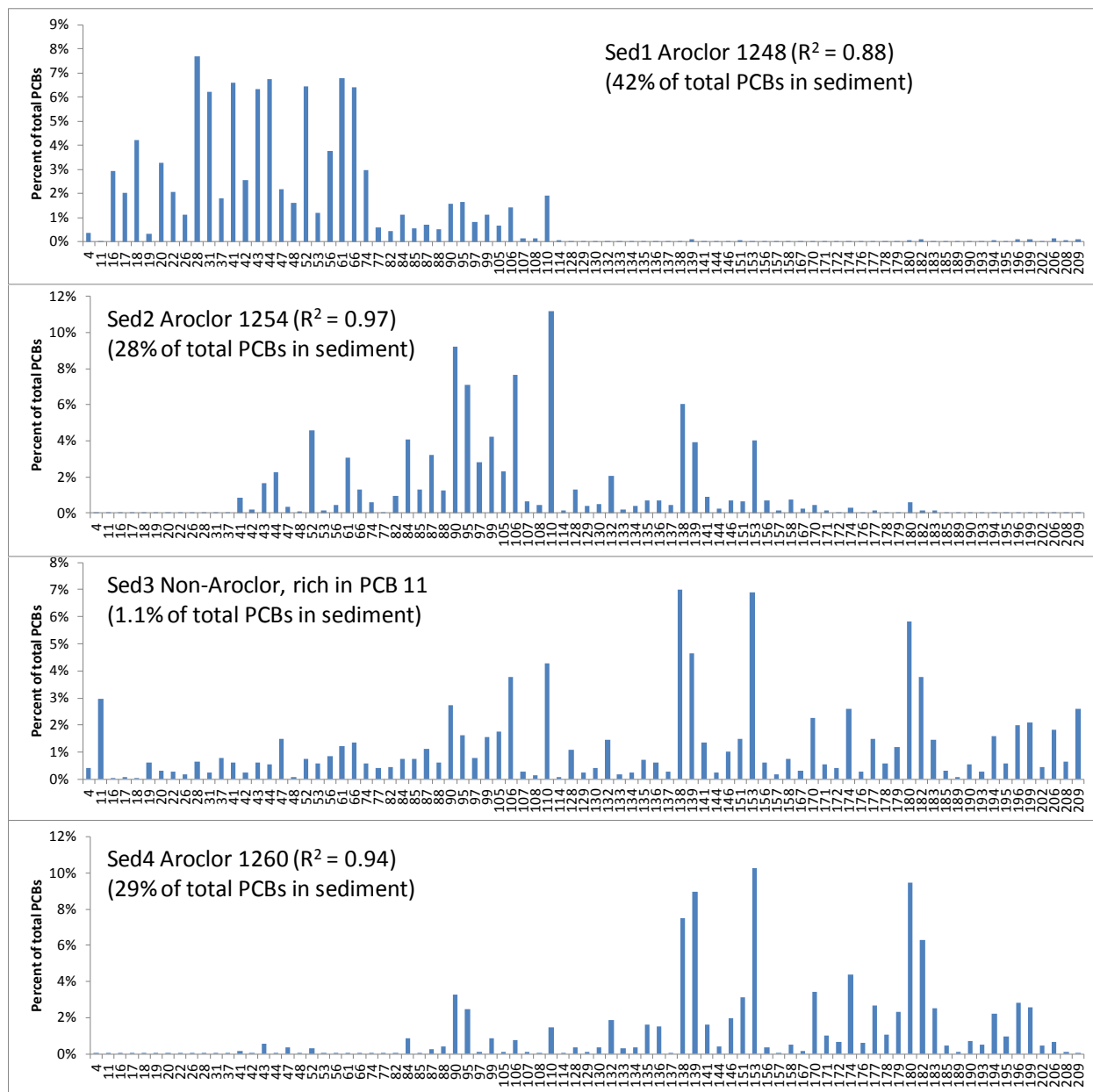


Figure S-3. Four factors resolved from the data matrix on PCBs in sediment.

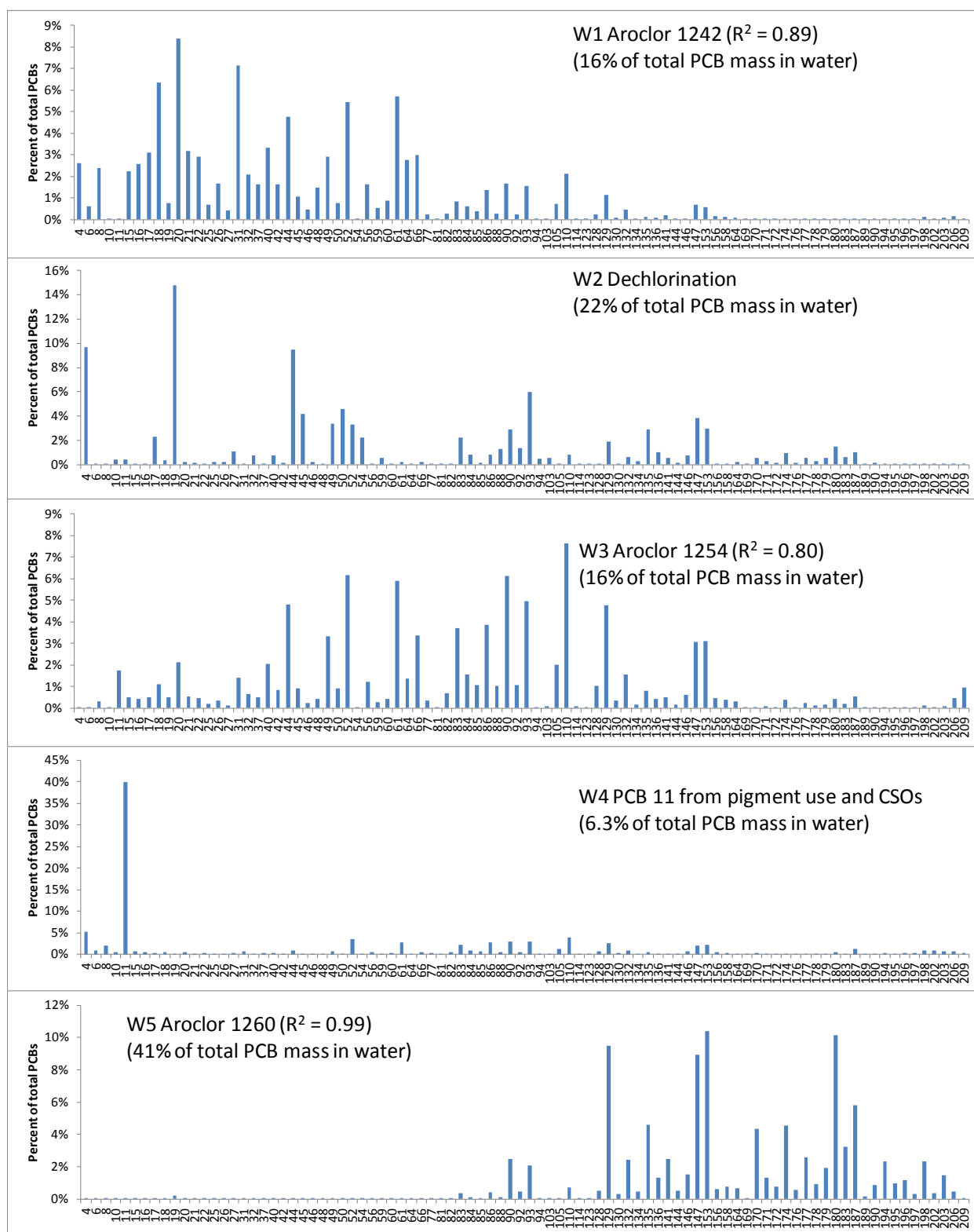


Figure S-4. Five factors resolved from the data set on PCBs in the water column.

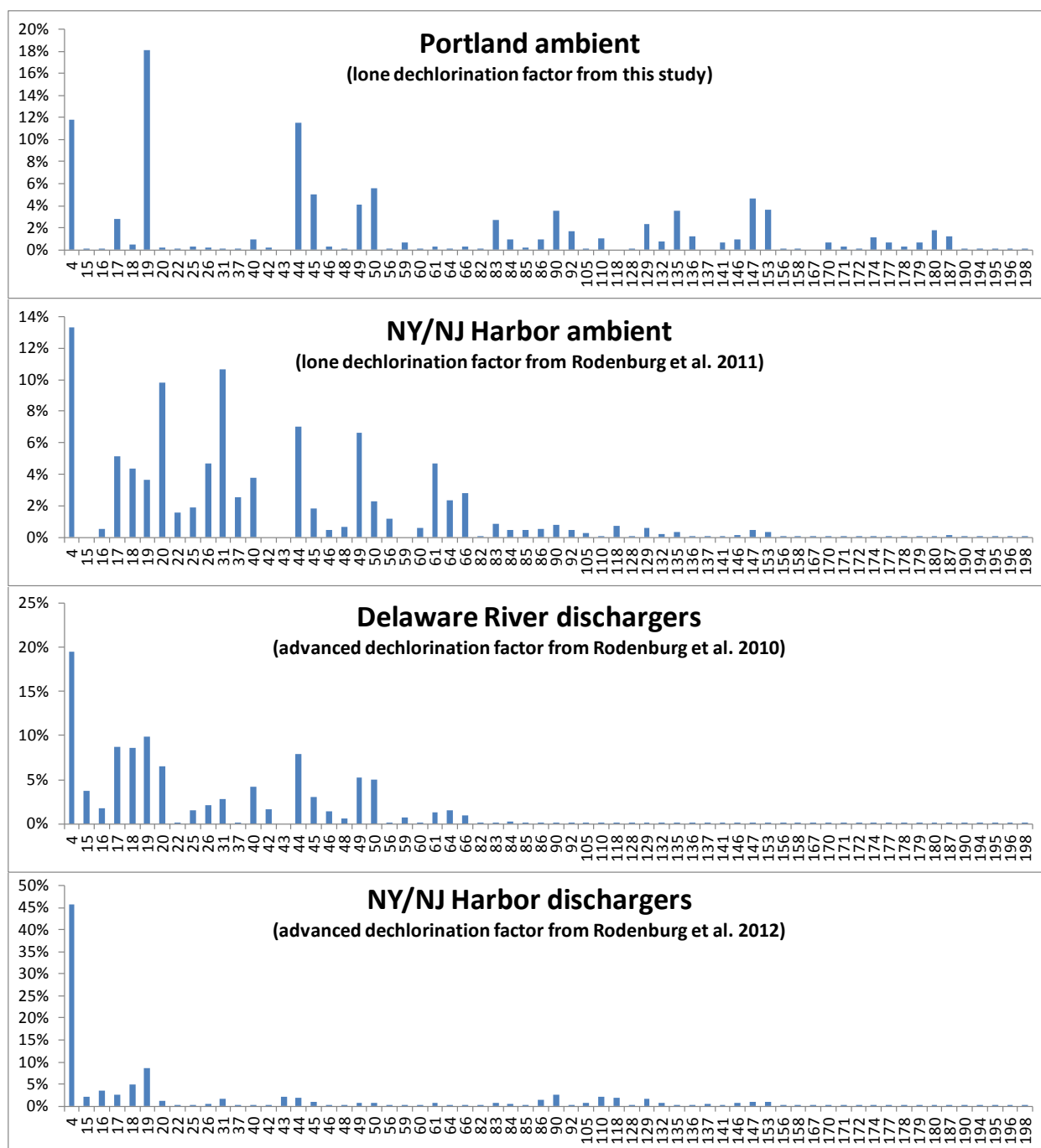


Figure S-6. Dechlorination factors resolved from factor analysis using various data sets. Because each data set utilized slightly different congener lists, only congeners common to all four data sets are shown. Note that co-eluting congeners are labeled using the lowest IUPAC congener number. All of these data sets utilized an SPB octyl GC column, so information about co-elutions is provided in Table S-1.